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On an exactly solvable model for quasi-bound states

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Abstract : An exactly solvable model which is similar to anharmonic oscillator in which the anharmonic term is negative, is given It is shown how to choose the correct boundary condition at $r \to \infty$ so that the quasibound state is of decaying type Explicit expressions for the real part of the complex energy and width are obtained when a parameter in the potential is taken to be large It is shown that the ordinary perturbation theory gives correct value of the real part of complex energy when the width of the state is small compared to the real part of the complex energy.

Keywords Decaying states

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In the study of atomic, molecular and nuclear physics, one frequently encounters quantum mechanical states which are not truly stationary. Examples are perturbed harmonic oscillator in which λx^4 is not positive [1,2] or the hydrogen atom perturbed by an electric field [3,4]. The exact wave function of such systems does not go to zero at infinity but becomes oscillatory at large distances. In the application of perturbation theory to such systems, one uses the unperturbed wave functions of bound state systems which give fairly accurate values of the perturbed state. The purpose of the present work is to construct an exactly solvable model for such problems and see under what conditions the perturbation theory should be expected to give fairly accurate results even though one is using the wave functions which do not satisfy the correct boundary conditions.

We describe the essential formulation in Section 2. The usual perturbative treatment will be given in Section 3. The concluding remarks are presented in Section 4.

The radial Schrödinger equation for the s wave is written as

$$-\frac{1}{2}\frac{d^2u}{dr^2} + V(r)\,u(r) = Eu(r), \tag{1}$$

where u satisfies the boundary condition $u(r) = 0$ at the origin $r = 0$.

Consider a potential $V(r)$ which is given by

$$V(r) = \frac{1}{2}r, \quad 0 \le r \le a, \tag{2a}$$

$$V(r) = -\frac{a}{2(b-a)}r + \frac{ab}{2(b-a)}, \quad r \ge a, \; b > a. \tag{2b}$$

Before we proceed to solve eq. (1) with the potential given by (2), we remark that potential (2) describes fairly well the situation, for example, of the anharmonic oscillator in which the anharmonic term is negative.

In the internal region $0 \le r \le a$, eq. (1) becomes

$$\frac{d^2u}{dr^2} - (r - 2E)u = 0. \tag{3}$$

The exact solution $u(r)$ of this equation is a linear combination of Airy's functions [5] Ai, Bi and is given by

$$u(r) = A\, Ai(r - 2E) + B\, Bi(r - 2E), \tag{4}$$

where A and B are constants. To determine the constants, one has to match this solution to the solution outside $r > a$. As the potential in the external region is given by (2b), this solution $u_E(r)$ is given by

$$u_E(r) = A_1 Ai\left[-\frac{1}{\lambda}\left(\frac{a}{b-a}r - \frac{ab}{b-a} + 2E\right)\right]$$
$$+ B_1 Bi\left[-\frac{1}{\lambda}\left(\frac{a}{b-a}r - \frac{ab}{b-a} + 2E\right)\right], \tag{5}$$

where $\lambda = \left(\frac{a}{b-a}\right)^{\frac{2}{3}}$ and A_1, B_1 are constants.

Let us now apply the boundary condition to (5) when $r \to \infty$. Using the asymptotic form for Ai, Bi, we find that one has to take

$$A_1 = iB_1, \tag{6}$$

if the solution is of outgoing type. With the relation (6), the asymptotic form of $u_E(r)$ is given by

$$u_E(r) \Rightarrow \pi^{-1/2}\left(-\frac{ar}{\lambda(b-a)}\right)^{-1/4} B_1 \exp$$

$$\exp \quad \frac{2\pi}{3} \quad \left(\lambda(b-a)\right)^{3/2} \tag{7}$$

The fact that this is the correct boundary condition will be confirmed later when we calculate the width Γ of the state. The sign of Γ will be such that it will imply a decaying state.

Matching the internal and external solutions at $r = a$ give

$$A\,Ai(a-2E) + B\,Bi(a-2E) = B_1\left[i\,Ai\left(\frac{1}{\lambda}(a-2E)\right) + Bi\left(\frac{1}{\lambda}(a-2E)\right)\right], \tag{6a}$$

$$A\,Ai'(a-2E) + B\,Bi'(a-2E) = -\frac{a}{\lambda(b-a)}B_1\left[iAi'\left(\frac{1}{\lambda}(a-2E)\right)\right.$$

$$\left.+\,Bi'\left(\frac{1}{\lambda}(a-2E)\right)\right]. \tag{6b}$$

The complex eigenvalue E is completely determined using above conditions (6) and the boundary condition at $r = 0$, which is given by

$$A\,Ai\,(-2E)+B\,Bi\,(-2E) = 0. \tag{7}$$

In order to find an explicit expression for the complex energy E, we take

$$b = a + a^2, \tag{8}$$

$a \gg 1$.

This is also the region for which perturbation theory works very well as will be shown later.

Using eqs. (6a), (6b) and (8) one can show that

$$\frac{B}{A} = \left(16a^{3/2}\right)^{-1}\exp\left(-\frac{4}{3}a^{3/2}\right) + \frac{i}{4}\exp\left(-\frac{4}{3}a^{5/2}\right). \tag{9}$$

Writing $E = \varepsilon_0 - i\Gamma$ and putting expression (9) in expression (7), we get for large values of a,

$$\varepsilon_0 = \frac{1}{2}x_0 - \frac{1}{2}\delta, \tag{10}$$

where, x_0 is the first zero of $Ai\,(-x) = 0$. Its value being 2.34. The quantity δ is given by

$$\delta = -\left(\frac{B}{A}\right)^r \frac{Bi(-x_0)}{Ai'(-x_0)}, \tag{11}$$

where $\left(\frac{B}{A}\right)^r$ is the real part of $\left(\frac{B}{A}\right)$.

The expression for the width Γ turns out to be

$$\Gamma = -\left(\frac{B}{A}\right)^i \frac{Bi(-2\varepsilon_0)}{2Ai'(-2\varepsilon_0)} \tag{12}$$

where $\left(\frac{B}{A}\right)^i$ is the imaginary part of $\left(\frac{B}{A}\right)$.

Since both $\left(\frac{B}{A}\right)'$ and $Ai'(-2\varepsilon_0)$ are positive while $Bi(-2\varepsilon_0)$ is negative, the width Γ is positive implying that the quasibound state is of decaying type. This shows that the boundary condition at $r \longrightarrow \infty$ is correctly chosen.

Another point to note is that the width Γ is much smaller than the real part ε of the complex energy.

In this section we would like to discuss the application of Rayleigh-Schrödinger perturbation theory to calculate the real part of the complex energy E using the unperturbed wave functions which satisfy the boundary condition at $r \longrightarrow \infty$ for the bound states. For this purpose we write the unperturbed hamiltonian H_0 as

$$H_0 = -\frac{1}{2}\frac{d^2}{dr^2} + \frac{1}{2}r, \quad 0 \le r \le \infty, \tag{13}$$

and the perturbation v as

$$\frac{a+1}{2a}(-r+a), \quad r \ge a. \tag{14}$$

The unperturbed ground state u_0 is then given by

$$u_0 = N\, Ai(r - x_0), \tag{15}$$

where N is the normalization constant.

The real part ε_0 of the complex energy E upto first order is then given by

$$\varepsilon_0 = \frac{1}{2}x_0 + \frac{a+1}{2a}\,\frac{\int_{r=0}^{\infty} dr\, Ai^2(r-x_0)(-r+a)}{\int_{r=0}^{\infty} dr\, Ai^2(r-x_0)}. \tag{16}$$

Taking a to be large as was done earlier, this gives

$$\varepsilon_0 = \frac{}{2}x_0 - \frac{}{32\pi}\left[\int_0 dr\, Ai^2(r-x_0)\right]^{-1} \exp\left(-\frac{4}{3}a^{3/2}\right) \tag{17}$$

Comparing (17) with the expression for ε_0 which is given by combining (9), (10), (11) we find that the dependence of ε_0 on the perturbation parameter a is the same in both the cases. Thus ordinary perturbation theory can be used to calculate the real part of the complex energy when the width Γ is small.

The exact eigenvalue of a quasibound state is given using a simplified form of the radial potential. The wave function satisfies the correct boundary condition at $r \longrightarrow \infty$ for a decaying state. This is confirmed by calculating the width of the state which shows that the state is of decaying type. By choosing a parameter in the potential to be large, algebraic expressions have been obtained for the real and imaginary parts of the complex energy. Using these results we have shown explicitly that ordinary perturbation theory gives the real part of the complex energy correctly even though in this calculation one uses unperturbed wave functions which satisfy the usual boundary condition of the bound states at infinity. This is the case where the width Γ of the decaying state is much smaller than the real part of the complex energy. What this implies is that the wave function over a large distance resembles to the one of the bound state problem.

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